FILE 'REGISTRY' ENTERED AT 14:43:44 ON 17 OCT 2007 Ll STRUCTURE UPLOADED L2 9894 S L1` L3 2 S L1 L4' 20 S L1 SSS FULL FILE 'CAPLUS' ENTERED AT 14:44:44 ON 17 OCT 2007 L5 35 S L4 FILE 'STNGUIDE' ENTERED AT 14:44:52 ON 17 OCT 2007 FILE 'HCAPLUS' ENTERED AT 14:47:13 ON 17 OCT 2007 L6 51792 S FLUORINAT? 909995 S (SACCHARIDE OR MONOSACCHARIDE OR NUCLEOSIDE OR RIBOS? OR GLUC L7 25 S L5 AND L6 L8 2 S L5 AND L6 AND L7 L9 FILE 'STNGUIDE' ENTERED AT 14:47:19 ON 17 OCT 2007 FILE 'HCAPLUS' ENTERED AT 14:47:41 ON 17 OCT 2007 FILE 'STNGUIDE' ENTERED AT 14:47:41 ON 17 OCT 2007 FILE 'HCAPLUS' ENTERED AT 14:49:18 ON 17 OCT 2007 12 S L8 AND (AY<2003 OR PY<2003 OR PRY<2003) L10

=> file registry
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 OCT 2007 HIGHEST RN 950817-67-1 DICTIONARY FILE UPDATES: 16 OCT 2007 HIGHEST RN 950817-67-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

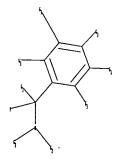
Please note that search-term pricing does apply when conducting SmartSELECT searches.

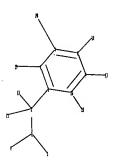
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10537437afterfinal.str





```
chain nodes :
1  2  3  4  11  13  16  17  18  19  20
ring nodes :
5  6  7  8  9  10
chain bonds :
1-2  1-3  1-4  2-5  2-11  2-13  6-19  7-20  8-16  9-17  10-18
ring bonds :
5-6  5-10  6-7  7-8  8-9  9-10
exact/norm bonds :
1-2  1-3  1-4  2-13  6-19  7-20  8-16  9-17  10-18
exact bonds :
2-5  2-11
normalized bonds :
5-6  5-10  6-7  7-8  8-9  9-10
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G1:H,Cl,Br,F,I

G2:CH3,CH2,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,H

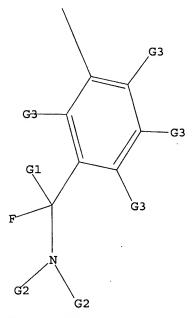
G3:H,CH3,Et,Cl,Br,F,I,MeO,NH2,NH3,NO2

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS

## L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



G1 H, Cl, Br, F, I

G2 Me,CH2, n-Pr,i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, Ph, H

G3 H, Me, Et, Cl, Br, F, I, MeO, NH2, NH3, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1` L2 9894 L1` ('L1')

=> s 11

SAMPLE SEARCH INITIATED 14:44:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 379 TO ITERATE

100.0% PROCESSED 379 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

6412 TO 8748 2 TO 124

PROJECTED ANSWERS:

2 SEA SSS'SAM L1

=> d 13 scan

L3

L3 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzenemethanamine, N, N-diethyl- $\alpha$ ,  $\alpha$ -diffuoro-2-methoxy-

MF C12 H17 F2 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzenemethanamine, N, N-diethyl- $\alpha$ ,  $\alpha$ -diffuoro-4-methoxy-

MF C12 H17 F2 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s ll sss full

FULL SEARCH INITIATED 14:44:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 7929 TO ITERATE

100.0% PROCESSED 7929 ITERATIONS

SEARCH TIME: 00.00.01

L4 20 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

20 ANSWERS

FULL ESTIMATED COST 177.50 177.71

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FILE COVERS 1907 - 17 Oct 2007 VOL 147 ISS 17 FILE LAST UPDATED: 16 Oct 2007 (20071016/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 14

L5 35 L4

=> file stnguide COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.47 178.18

FILE 'STNGUIDE' ENTERED AT 14:44:52 ON 17 OCT 2007 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION. LAST RELOADED: Oct 12, 2007 (20071012/UP).

=> file hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 178.42 0.24

FULL ESTIMATED COST

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FILE COVERS 1907 - 17 Oct 2007 VOL 147 ISS 17 FILE LAST UPDATED: 16 Oct 2007 (20071016/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s fluorinat?

=> s (saccharide or monosaccharide or nucleoside or ribos? or glucos? or fructos? or arabons? or fucos? or (N-acetylglucosamin?) or (N-acetylgalactosamin?) or sugar)

10271 SACCHARIDE

11905 MONOSACCHARIDE

48930 NUCLEOSIDE

120294 RIBOS?

514419 GLUCOS?

70340 FRUCTOS?

0 ARABONS?

19142 FUCOS?

3094512 N

18895 ACETYLGLUCOSAMIN?

16088 N-ACETYLGLUCOSAMIN?

(N(W) ACETYLGLUCOSAMIN?)

3094512 N

6208 ACETYLGALACTOSAMIN?

5570 N-ACETYLGALACTOSAMIN?

(N(W) ACETYLGALACTOSAMIN?)

268138 SUGAR

L7 909995 (SACCHARIDE OR MONOSACCHARIDE OR NUCLEOSIDE OR RIBOS? OR GLUCOS?
OR FRUCTOS? OR ARABONS? OR FUCOS? OR (N-ACETYLGLUCOSAMIN?) OR

(N-ACETYLGALACTOSAMIN?) OR SUGAR)

=> s 15 and 16

35 L4

L8 25 L5 AND L6

=> s 15 and 16 and 17

35 L4

L9 2 L5 AND L6 AND L7

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

2.60

181.02

FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 14:47:19 ON 17 OCT 2007 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Oct 12, 2007 (20071012/UP).

=> d 19 1-2 ti abs bib

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y) /N:y

- L9 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
- TI Deoxyfluorination of alcohols using N,N-diethyl- $\alpha$ ,  $\alpha$ -difluoro-(m-methylbenzyl)amine
- AB Deoxyfluorination of alcs. was carried out using N,N-diethyl-  $\alpha,\alpha$ -difluoro-(m-methylbenzyl)amine (DFMBA). Primary alcs. were effectively converted to fluorides under microwave irradiation or conventional heating. Deoxyfluorination of an anomeric hydroxy group in sugars by DFMBA proceeded at below room temperature and glycosyl fluorides could

be obtained in good yields. The deoxyfluorination reaction

chemoselectively proceeded and various protecting groups on the sugar can survive under the reaction conditions. ΑN 2004:581849 HCAPLUS <<LOGINID::20071017>> DN141:260951 Deoxyfluorination of alcohols using N,N-diethyl-α,α-difluoro-ΤI (m-methylbenzyl)amine Kobayashi, Shingo; Yoneda, Atushi; Fukuhara, Tsuyoshi; Hara, Shoji AU Division of Molecular Chemistry, Graduate School of Engineering, Hokkaido CS University, Sapporo, 060-8628, Japan Tetrahedron (2004), 60(32), 6923-6930 SO CODEN: TETRAB; ISSN: 0040-4020 PB Elsevier Science B.V. DT Journal LA English OS CASREACT 141:260951 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN L9 Method of fluorination using N, N-diethyl- $\alpha$ ,  $\alpha$ difluorobenzylamines Disclosed is a method in which a glucide, examples of which include a AB monosaccharide, an oligosaccharide, a polysaccharide, a composite saccharide comprising any of these saccharides and a protein or lipid bonded thereto, a polyalc., an aldehyde, ketone, or acid of a polyalc., a derivative or condensate of any of these, is reacted with a fluorinating agent represented by the general formula of RCF2-Y(R1)R2 [y = N, P; R-R2 are same or different group selected from H and each (un) substituted alkyl and aryl; or ≥2 of R-R2 groups are bonded to each other to form a ring] either thermally or by irradiation with microwave or an electromagnetic wave with a wavelength around the microwave region. By the method, fluorination reaction can be safely conducted position-selectively even in a temperature range of 150 to 200°, in which fluorination has conventionally been difficult. The method in which the reactants are irradiated with microwave or an electromagnetic wave with a wavelength around the microwave region is applicable to substrates other than glucides. When a complex compound comprising HF and a base, for example, is reacted with a substrate by irradiation with microwave, fluorination in a specific position which has been difficult in conventional techniques proceeds highly selectively in a short time efficiently and safely. Thus, 10 mmol Me 2,3-O-isopropylidene- $\beta$ -D-ribofuranoside, 12 mmol N, N-diethyl- $\alpha$ ,  $\alpha$ -difluoro-3-methylbenzylamine, and 20 mL heptane were added to a glass vessel reaction vessel coated with fluorinated resin, heated with 100° with stirring, and allowed to react for 50 min to give 55% Me 2,3-O-isopropylidene-5-deoxy-5fluoro- $\beta$ -D-ribofuranoside. 2004:493719 HCAPLUS <<LOGINID::20071017>> ΑN DN 141:38808 TI Method of fluorination using N,N-diethyl- $\alpha$ , $\alpha$ difluorobenzylamines Hara, Shoji; Fukuhara, Tsuyoshi IN Mitsubishi Gas Chemical Company, Inc., Japan PA SO PCT Int. Appl., 50 pp. CODEN: PIXXD2 DT Patent LA Japanese FAN.CNT 1 PATENT NO. KIND APPLICATION NO. DATE DATE --------------------WO 2004050676 WO 2003-JP15336 PΙ A1 20040617 20031201 W: CN, US RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,

IT, LU, MC, NL, PT, RO, SE, SI, SK, TR

|       | JР           | 2004182664 |       |       |      |      |             | 2004 | 0702 | JP     | 2002-  | 35296    | 8    |      | 20    | 021: | 204 |
|-------|--------------|------------|-------|-------|------|------|-------------|------|------|--------|--------|----------|------|------|-------|------|-----|
|       | JP           | 2004189655 |       |       |      |      |             | 2004 | 0708 | JP     | 20     | 20021210 |      |      |       |      |     |
|       | ΕP           | 1568703    |       |       |      | A1   | A1 20050831 |      |      | EP     | •      | 20031201 |      |      |       |      |     |
|       |              | R:         | AT,   | BE,   | CH,  | DE,  | DK,         | ES,  | FR,  | GB, G  | R, IT, | LI,      | LU,  | NL,  | SE,   | MC,  | PT, |
|       |              |            | ΙE,   | SI,   | FI,  | RO,  | CY,         | TR,  | BG,  | CZ, E  | E, HU, | SK       |      |      |       |      |     |
|       | CN           | 17202      | 256   |       |      | Α    |             | 2006 | 0111 | CN     | 2003-  | -80104   | 1679 |      | 20    | 031: | 201 |
|       | CN           | 1974       | 588   |       |      | Α    |             | 2007 | 0606 | CN     | 2006-  | -10164   | 1022 |      | 20    | 031: | 201 |
|       | US           | 2006       | 0149  | 72    |      | A1   |             | 2006 | 0119 | US     | 2005-  | -53743   | 37   |      | 20    | 050  | 503 |
| PRAI  | JP           | 2002       | -3529 | 968   |      | Α    |             | 2002 | 1204 |        |        |          |      |      |       |      |     |
|       | JP           | 2002       | -3582 | 249   |      | Α    |             | 2002 | 1210 |        |        |          |      |      |       |      |     |
|       | CN           | 2003       | -801  | 0467  | 9    | A3   | }           | 2003 | 1201 |        |        |          |      |      |       |      |     |
|       | WO           | 2003       | -JP1  | 5336  |      | W    |             | 2003 | 1201 |        |        |          |      |      |       |      |     |
| os    | CAS          | REAC'      | r 14: | 1:388 | 308; | MAF  | RPAT        | 141: | 3880 | 3      |        |          |      |      |       |      |     |
| RE.CI | $\mathbf{T}$ | 19         | THI   | ERE A | ARE  | 19 ( | CITED       | REF  | EREN | CES AV | AILABI | LE FOR   | R TH | IS R | ECORI | )    |     |

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file hcaplus COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 0.18 189.52 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -1.56

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FILE COVERS 1907 - 17 Oct 2007 VOL 147 ISS 17 FILE LAST UPDATED: 16 Oct 2007 (20071016/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 18 and (AY<2003 or PY<2003 or PRY<2003)

4465265 AY<2003 22908103 PY<2003 3944043 PRY<2003 12 L8 AND (AY<2003 OR PY<2003 OR PRY<2003)

=> file stnguide

L10

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 2.60 192.12 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

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LAST RELOADED: Oct 12, 2007 (20071012/UP).

=> d 110 1-12 ti abs bib hitstr
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L10 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of fluorinated alicyclic compounds using difluoroamines as thermally stable safe fluorination agents

AB In title process, R0CF2NR1R2 [R0-R2 = H, (un)substituted alkyl, aryl; ≥2 of them may be linked to form ring] are used. Thus, Me 3-hydroxyadamantane-1-carboxylate was fluorinated with 3-MeC6H4CF2NEt2 at room temperature for 14 h to give 98% Me

3-fluoroadamantane-1-carboxylate.

AN 2004:529739 HCAPLUS <<LOGINID::20071017>>

DN 141:88875

TI Preparation of fluorinated alicyclic compounds using difluoroamines as thermally stable safe fluorination agents

IN Kawai, Ken; Fushimi, Norio; Hidaka, Toshio

PA Mitsubishi Gas Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 13 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

|      | PATENT NO.  | KIND     | DATE       | APPLICATION NO.          | DATE         |  |  |  |  |  |  |  |  |
|------|---|----------|------------|--------------------------|--------------|--|--|--|--|--|--|--|--|
|      |   |          |            |                          |              |  |  |  |  |  |  |  |  |
| PΙ   | JP 2004182671   | A        | 20040702   | JP 2002-353469           | 20021205 <   |  |  |  |  |  |  |  |  |
| PRAI | JP 2002-353469  |          | 20021205 < |                          |              |  |  |  |  |  |  |  |  |
| OS   | MARPAT 141:88875  |          |            |                          |              |  |  |  |  |  |  |  |  |
| IT   | 500131-50-0P, N,N-Diethyl-α,α-difluoro-(3-                            |          |            |                          |              |  |  |  |  |  |  |  |  |
|      | methyl) benzylamine 704916-04-1P, N, N-Diethyl- $\alpha$ , $\alpha$ - |          |            |                          |              |  |  |  |  |  |  |  |  |
|      | difluoro-(2-methoxy   | ) benzyl | amine      | -                        | •            |  |  |  |  |  |  |  |  |
|      |   |          |            | paration); PREP (Prepara | ation); RACT |  |  |  |  |  |  |  |  |
|      | (Reactant or reagen   |          |            |                          |              |  |  |  |  |  |  |  |  |

(fluorination of alicyclic compds. with thermally stable safe difluoroamines)

RN 500131-50-0 HCAPLUS

CN Benzenemethanamine, N,N-diethyl- $\alpha$ , $\alpha$ -difluoro-3-methyl- (CA INDEX NAME)

RN 704916-04-1 HCAPLUS

CN Benzenemethanamine, N,N-diethyl- $\alpha$ , $\alpha$ -difluoro-2-methoxy- (CA INDEX NAME)

```
L10 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
     Preparation of thermally stable fluorination agents and
     fluorination of functional group-containing compounds with them
     Substrates are fluorinated with ROCF2NR1R2 [RO-R2 = H,
AB
     (un) substituted alkyl, aryl; ≥2 of them may be linked to form
     ring]. Thus, fluorination of N,N-diethyl-\alpha-chloro-(2-
     methoxyphenyl)amidium chloride with KF at 80° for 20 h gave 55%
     2-MeOC6H4CF2NEt2, with which 1-adamantanol was fluorinated at
     60° for 14 h to afford 86% 1-fluoroadamantane.
     2004:529733 HCAPLUS <<LOGINID::20071017>>
AN
     141:53982
DN
     Preparation of thermally stable fluorination agents and
TI
     fluorination of functional group-containing compounds with them
     Yamada, Kazuhiro; Hidaka, Toshio
IN
PΑ
     Mitsubishi Gas Chemical Co., Ltd., Japan
     Jpn. Kokai Tokkyo Koho, 9 pp.
SO
     CODEN: JKXXAF
DT
     Patent
LA
     Japanese
FAN.CNT 1
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                                            JP 2002-353010
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                         Α
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PRAI JP 2002-353010
                                20021204
                                         <--
     MARPAT 141:53982
os
     704916-04-1P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (fluorination of functional group-containing compds. with
```

Benzenemethanamine, N, N-diethyl-α, α-difluoro-2-methoxy- (CA

INDEX NAME)

RN

CN

- L10 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
- TI Method of fluorination using N,N-diethyl- $\alpha$ , $\alpha$ -difluorobenzylamines

thermally stable difluoroamines)

704916-04-1 HCAPLUS

Disclosed is a method in which a glucide, examples of which include a monosaccharide, an oligosaccharide, a polysaccharide, a composite saccharide comprising any of these saccharides and a protein or lipid bonded thereto, a polyalc., an aldehyde, ketone, or acid of a polyalc., a derivative or condensate of any of these, is reacted with a fluorinating agent represented by the general formula of RCF2-Y(R1)R2 [y = N, P; R-R2 are same or different group selected from H and each (un)substituted alkyl and aryl; or ≥2 of R-R2 groups are bonded to each other to form a ring] either thermally or by irradiation with microwave or an electromagnetic wave with a wavelength around the

```
microwave region. By the method, fluorination reaction can be
     safely conducted position-selectively even in a temperature range of 150 to
     200°, in which fluorination has conventionally been
     difficult. The method in which the reactants are irradiated with
     microwave or an electromagnetic wave with a wavelength around the
     microwave region is applicable to substrates other than glucides.
     complex compound comprising HF and a base, for example, is reacted with a
     substrate by irradiation with microwave, fluorination in a specific
     position which has been difficult in conventional techniques proceeds
     highly selectively in a short time efficiently and safely. Thus, 10 mmol
     Me 2,3-0-isopropylidene-\beta-D-ribofuranoside, 12 mmol
     N, N-diethyl-\alpha, \alpha-difluoro-3-methylbenzylamine, and 20 mL
     heptane were added to a glass vessel reaction vessel coated with
     fluorinated resin, heated with 100° with stirring, and
     allowed to react for 50 min to give 55% Me 2,3-O-isopropylidene-5-deoxy-5-
     fluoro-\beta-D-ribofuranoside.
     2004:493719 HCAPLUS <<LOGINID::20071017>>
     141:38808
     Method of fluorination using N,N-diethyl-\alpha,\alpha-
     difluorobenzylamines
     Hara, Shoji; Fukuhara, Tsuyoshi
     Mitsubishi Gas Chemical Company, Inc., Japan
     PCT Int. Appl., 50 pp.
     CODEN: PIXXD2
     Patent
     Japanese
FAN.CNT 1
     PATENT NO.
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                                            APPLICATION NO.
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     WO 2004050676
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                                20021204
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     JP 2002-358249
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                                20021210 <--
     CN 2003-80104679
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                                20031201
     WO 2003-JP15336
                          W
                                20031201
     CASREACT 141:38808; MARPAT 141:38808
     500131-50-0P, N, N-Diethyl-\alpha, \alpha-difluoro-3-
     methylbenzylamine 704916-04-1P, N,N-Diethyl-\alpha,\alpha-
     difluoro-2-methoxybenzylamine
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (fluorination agent; preparation of N,N-diethyl-\alpha,\alpha-
        difluorobenzylamines as fluorinating agents for
        monosaccharides, alcs., ketones, epoxides, and aldehydes)
     500131-50-0 HCAPLUS
     Benzenemethanamine, N, N-diethyl-\alpha, \alpha-difluoro-3-methyl- (CA
     INDEX NAME)
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AN DN

TI

IN

PA

SO

DT

LА

PΙ

OS

RN

CN

704916-04-1 HCAPLUS RN

Benzenémethanamine, N,N-diethyl-α,α-difluoro-2-methoxy-(CA CN INDEX NAME)

## THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 19 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

Fluorination under microwave irradiation TI

Substrates are fluorinated by fluoro compds. under (near-)microwave irradiation 1-Dodecanol was fluorinated by AB N, N-diethyl- $\alpha, \alpha$ -difluoro-3-methylbenzylamine under microwave irradiation at room temperature for 10 min to give 93% 1-fluorododecane.

2004:330166 HCAPLUS <<LOGINID::20071017>> ΑN

140:338752 DN

Fluorination under microwave irradiation TI

Hara, Masaharu; Fukuhara, Katashi IN

Mitsubishi Gas Chemical Co., Ltd., Japan PA

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DTPatent

Japanese LΑ

FAN.CNT 1

| PATENT NO.                              | KIND        | DATE         | APPLICATION NO. | DATE         |
|---|-------------|--------------|-----------------|--------------|
|   |             | 20040422     | JP 2002-290198  | 20021002 <   |
| PI JP 2004123605<br>PRAI JP 2002-290198 | A           | 20040422     |                 | 20021002 255 |
| OS CASREACT 140:33                      | OTET. MADD  |              | -               |              |
| IT 500131-50-0                          | 00/52; MARP | 41 140:33673 | <i>52</i> .     |              |
| RL: RCT (Reacta                         | nt): RACT   | (Reactant of | r reagent)      |              |

microwave irradiation) RN500131-50-0 HCAPLUS

Benzenemethanamine, N,N-diethyl- $\alpha$ , $\alpha$ -difluoro-3-methyl-CN INDEX NAME)

(fluorination of organic compds. by fluoro amines under

L10 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

Preparation of heat-stable fluorine compounds, fluorination TI agents thereof, and surface treatment agents, cleaning solvents, and coatings containing them

ROCF2XR1R2 [X = N, P; RO, R1, R2 = H, (un) substituted alkyl, aryl; RO, R1, ABR2 may be linked to form ring] are prepared Also claimed are ROCY:X+R1R2 Y-(X, R0-R2 = same as above; Y = Cl, Br, I) as the intermediates of the F compds. Thus, 3-MeC6H4CCl:N+Et2 Cl- was refluxed with KF in MeCN for 18 h to give .apprx.60% 3-MeC6H4CF2NEt2, which was stable when heated at 200° for 1 h in a sealed tube. Fluorination of PhCH2OH

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with 3-MeC6H4CF2NEt2 gave 100% PhCH2F. 2003:165059 HCAPLUS <<LOGINID::20071017>>
```

DN 138:204826

AN

TI Preparation of heat-stable fluorine compounds, fluorination agents thereof, and surface treatment agents, cleaning solvents, and coatings containing them

IN Hidaka, Toshio; Fushimi, Norio; Yoshimura, Takashi; Kawai, Takeshi

PA Mitsubishi Gas Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

|    |     | -111          | _             |      |      |      |             |             |      |                |                |                 |      |      |     |              |            |       |     |   |  |
|----|-----|---------------|---------------|------|------|------|-------------|-------------|------|----------------|----------------|-----------------|------|------|-----|--------------|------------|-------|-----|---|--|
|    |     | PAT           | TENT          | NO.  |      |      | KINI        | ) :         | DATE |                |                | APPLICATION NO. |      |      |     |              | DATE       |       |     |   |  |
|    |     |               |               |      |      |      |             | -           |      |                |                |                 |      |      |     |              |            |       |     |   |  |
| P: | I   | JР            | JP 2003064034 |      |      |      |             |             | 2003 | 0305           | JP 2001-257833 |                 |      |      |     |              | 20010828 < |       |     |   |  |
|    |     | WO            | WO 2003020685 |      |      |      |             | 20030313    |      |                | WO 2002-JP8477 |                 |      |      |     | . 20020822 < |            |       |     |   |  |
|    |     | W: US         |               |      |      |      |             |             |      |                |                |                 |      |      |     |              |            |       |     |   |  |
|    |     |               | RW:           | AT,  | BE,  | BG,  | CH,         | CY,         | CZ,  | DE,            | DK,            | EE,             | ES,  | FI,  | FR, | GB,          | GR,        | ΙE,   | IT, |   |  |
|    |     |               |               | LU,  | MC,  | NL,  | PT,         | SE,         | SK,  | TR             |                |                 |      |      |     |              |            |       |     |   |  |
|    |     | EP 1422216    |               |      |      |      | A1 20040526 |             |      | EP 2002-760710 |                |                 |      |      |     | 20020822 <   |            |       |     |   |  |
|    |     |               | R:            | ΑT,  | ΒE,  | CH,  | DE,         | DK,         | ES,  | FR,            | GB,            | GR,             | IT,  | LI,  | LU, | NL,          | SE,        | MC,   | PT, |   |  |
|    |     |               |               | ΙE,  | FI,  | CY,  | TR,         | BG,         | CZ,  | EE,            | SK             |                 |      |      |     |              |            |       |     |   |  |
|    |     | US 2004073065 |               |      |      |      | Al          | A1 20040415 |      |                | US 2003-433412 |                 |      |      |     | 20030604 <   |            |       |     |   |  |
|    |     | US            | 7019          | 173  |      |      | B2          |             | 2006 | 0328           |                |                 |      |      |     |              |            |       |     |   |  |
|    |     | US            | 2006          | 0895 | 13   |      | A1          |             | 2006 | 0427           | 1              | JS 2            | 005- | 2974 | 8 0 |              | 20         | 00512 | 209 | < |  |
| P  | RAI | JP            | 2001          | -257 | 833  |      | Α           |             | 2001 | 0828           | <              | -               |      |      |     |              |            |       |     |   |  |
|    |     | WO            | 2002          | -JP8 | 477  |      | W           |             | 2002 | 0822           | <              | -               |      |      |     |              |            |       |     |   |  |
|    |     | US            | 2003          | -433 | 412  |      | <b>A</b> 3  |             | 2003 | 0604           |                |                 |      |      |     |              |            |       |     |   |  |
| 0  | S   | CAS           | SREAC         | T 13 | 8:20 | 4826 | ; MAI       | RPAT        | 138  | :204           | 826            |                 |      |      |     |              |            |       |     |   |  |
| ľ  | Т   | 500           | 131-          | 50-0 | P    |      |             |             |      |                |                |                 |      |      |     |              |            |       |     |   |  |

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(fluorination agent; preparation of heat-stable F compds. via amidium halides for fluorination agents, surface treatment agents, cleaning solvents, and coatings)

RN 500131-50-0 HCAPLUS

CN Benzenemethanamine, N,N-diethyl- $\alpha$ , $\alpha$ -difluoro-3-methyl- (CA INDEX NAME)

L10 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Fluorination of thiocarbonyl compounds with bis(2methoxyethyl)aminosulfur trifluoride (Deoxo-Fluor reagent): a facile synthesis of gem-difluorides

AB A variety of thiocarbonyl derivs. (thioketone, thioester, thioamide, dithioester, and dithiocarbamate) were converted to the corresponding gem-difluorides in excellent yields on reaction with the fluorinating agent, bis(2-methoxyethyl)aminosulfur trifluoride (I), in the presence of SbCl3. Thus, reacting PhC(S)Ph with I gave PhCF2Ph in 89% yield.

AN 2000:463617 HCAPLUS <<LOGINID::20071017>>

DN 133:192747

TI Fluorination of thiocarbonyl compounds with bis(2methoxyethyl)aminosulfur trifluoride (Deoxo-Fluor reagent): a facile

```
synthesis of gem-difluorides
     Lal, Gauri S.; Lobach, Elyse; Evans, Ann
ΑU
     Air Products and Chemicals Inc., Allentown, PA, 18195-1501, USA
CS
     Journal of Organic Chemistry (2000), 65(16), 4830-4832
SO
     CODEN: JOCEAH; ISSN: 0022-3263
PB
     American Chemical Society
     Journal
DT
LA
     English
os
     CASREACT 133:192747
IT
     702-99-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of gem-difluorides by fluorination of thiocarbonyl
        compds. with Deoxo-Fluor reagent)
     702-99-8 HCAPLUS
RN
     Benzenemethanamine, α,α-difluoro-N,N-dimethyl- (CA INDEX
CN
     NAME)
Ph-CF2-NMe2
RE.CNT
        36
              THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L10
    ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
     Reactions of N,N-dialkylbenzamides with sulfur tetrafluoride.
TI
     of dialkyl-\alpha, \alpha-difluorobenzylamines
     The KF-catalyzed reaction of amides R2NCOC6H4R1 (I; R = Me, Et, Pr,
AB
     CH2CH2CF3; R1 = H, Me, OMe, Br, CF3, NO2) with SF4 gave amines
     R2NCF2C6H4R1. Substituent effects of the R1 in I (R = Me) is discussed.
     AN
DN
     100:209316
     Reactions of N,N-dialkylbenzamides with sulfur tetrafluoride.
ΤI
     of dialkyl-\alpha, \alpha-difluorobenzylamines
     Dmowski, Wojciech; Kaminski, Maciej
ΑU
     Inst. Org. Chem., Pol. Acad. Sci., Warsaw, 01224, Pol.
CS
     Polish Journal of Chemistry (1982), 56(10-12), 1369-78
SO
     CODEN: PJCHDQ; ISSN: 0137-5083
     Journal
DT
     English
LA
os
     CASREACT 100:209316.
     702-99-8P 90238-11-2P 90238-12-3P
IT
     90238-13-4P 90238-14-5P 90238-15-6P
     90238-18-9P 90238-20-3P 90238-21-4P
     90238-22-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     702-99-8 HCAPLUS
RN
     Benzenemethanamine, \alpha, \alpha-difluoro-N, N-dimethyl-
                                                      (CA INDEX
CN
     NAME)
Ph-CF2-NMe2
RN
     90238-11-2 HCAPLUS
     Benzenemethanamine, \alpha, \alpha-difluoro-N, N, 4-trimethyl- (9CI)
CN
     INDEX NAME)
```

$$CF_2-NMe_2$$

RN 90238-12-3 HCAPLUS

CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-N,N,3-trimethyl- (9CI) (CA INDEX NAME)

RN 90238-13-4 HCAPLUS

CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-4-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 90238-14-5 HCAPLUS

CN Benzenemethanamine, 4-bromo- $\alpha$ ,  $\alpha$ -difluoro-N, N-dimethyl- (9CI) (CA INDEX NAME)

RN 90238-15-6 HCAPLUS

CN Benzenemethanamine, 3-bromo- $\alpha$ ,  $\alpha$ -difluoro-N, N-dimethyl- (9CI) (CA INDEX NAME)

RN 90238-18-9 HCAPLUS

CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-N,N-dimethyl-4-nitro- (9CI) (CA INDEX NAME)

RN 90238-20-3 HCAPLUS

CN Benzenemethanamine, N,N-diethyl- $\alpha$ , $\alpha$ -difluoro- (9CI) (CA INDEX NAME)

Ph-CF2-NEt2

RN 90238-21-4 HCAPLUS

CN Benzenemethanamine,  $\alpha$ ,  $\alpha$ -difluoro-N, N-dipropyl- (9CI) (CA INDEX NAME)

 $Ph-CF_2-N(Pr-n)_2$ 

RN 90238-22-5 HCAPLUS

CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-N,N-bis(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Dialkyl- $\alpha$ ,  $\alpha$ -difluorobenzylamines and

dialkyl(trifluoromethyl)amines - novel fluorinating reagents

AB The use of PhCF2NMe2 and CF3NEt2 as fluorinating reagents to replace OH groups in alcs. and carboxylic acids by F has been studied. The results, which are very variable, are compared with those reported for other fluoroamine reagents.

AN 1984:34109 HCAPLUS <<LOGINID::20071017>>

DN 100:34109

.TI Dialkyl- $\alpha$ ,  $\alpha$ -difluorobenzylamines and dialkyl(trifluoromethyl)amines - novel fluorinating reagents

AU Dmowski, Wojciech; Kaminski, Maciej

CS Inst. Org. Chem., Pol. Acad. Sci., Warsaw, 00-961, Pol.

SO Journal of Fluorine Chemistry (1983), 23(3), 219-28 CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

OS CASREACT 100:34109

IT 702-99-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of alcs. and carboxylic acids by)

RN 702-99-8 HCAPLUS

CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-N,N-dimethyl- (CA INDEX NAME)

- L10 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthetic methods and reactions. I. Seleniuum tetrafluoride and its pyridine complex. Convenient fluorinating agents for fluorination of ketones, aldehydes, amides, alcohols, carboxylic acids, and anhydrides
- AB Selenium tetrafluoride is a general purpose, convenient fluorinating agent for a wide variety of compds., such as ketones, aldehydes, amides, alcs., carboxylic acids, and anhydrides. Addition of pyridine, which forms a complex with SeF4, in fluorination of alcs. generally prevents isomerization and allows preparation of primary fluorides.
- AN 1974:81959 HCAPLUS <<LOGINID::20071017>>
- DN 80:81959
- TI Synthetic methods and reactions. I. Seleniuum tetrafluoride and its pyridine complex. Convenient fluorinating agents for fluorination of ketones, aldehydes, amides, alcohols, carboxylic acids, and anhydrides
- AU Olah, George A.; Nojima, Masatomo; Kerekes, Istvan
- CS Dep. Chem., Case West. Reserve Univ., Cleveland, OH, USA
- SO Journal of the American Chemical Society (1974), 96(3), 925-7 CODEN: JACSAT; ISSN: 0002-7863
- DT Journal
- LA English
- IT 702-99-8P
- RN 702-99-8 HCAPLUS
- CN Benzenemethanamine,  $\alpha, \alpha$ -difluoro-N,N-dimethyl- (CA INDEX NAME)

Ph-CF2-NMe2

- L10 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
- TI Chemistry of carbonyl fluoride. I. Fluorination of organic compounds
- Carbonyl fluoride reacts with carbonyl compds. such as cyclohexanone, benzaldehyde, and benzophenone to give the gem-difluorides, while HCONMe2 yields  $\alpha, \alpha$ -difluorotrimethylamine. Metal fluoride-catalyzed addition at the ethylenic bond in perfluoro olefins forms perfluoroacyl fluorides, while the C-N unsatd, compds. CF3N: CF2, PhNCO, and CF3CN give, resp., (CF3)2NCOF, PhN(COF)2, and CF3CF2NCO. The exptl. technique, infrared and nuclear magnetic resonance spectra are given.
- AN 1963:66175 HCAPLUS <<LOGINID::20071017>>
- DN 58:66175
- OREF 58:11243a-b
- TI Chemistry of carbonyl fluoride. I. Fluorination of organic compounds
- AU Fawcett, F. S.; Tullock, C. W.; Coffman, D. D.
- CS E. I. du Pont de Nemours Co., Wilmington, DE
- SO Journal of the American Chemical Society (1962), 84, 4275-85 CODEN: JACSAT; ISSN: 0002-7863
- DT Journal
- LA Unavailable
- OS CASREACT 58:66175
- IT 702-99-8P, Benzylamine,  $\alpha, \alpha$ -difluoro-N, N-dimethyl-

```
Ph-CF2-NMe2
     ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
L10
     Fluorinated organic compounds
TI
     The title compds. can be used as chemical intermediates. Cyclohexanone 40,
     COF2 65, and HCONMe2 4-5 parts are placed in a reactor containing N, the
     reactor is closed, the mixture heated at 50° 12 hrs. under autogenous
     pressure, cooled, the volatile materials are removed, and the remaining
     liquid is distilled to give 1-fluorocyclohexyl fluoroformate (I), b27
     59-63°, 52 parts. I 17, hexane 30-5, and BF3-etherate 4.8 parts
     are heated at 45-7° 3 hrs., the mixture is cooled, the upper phase
     separated, agitated with powdered NaF, the NaF filtered off, the filtrate
evaporated,
     and the residue distilled through a fractionating column to give
     1,1-di-fluorocyclohexane, b. 101-7°, n25D 1.3900-1.3895, 5.6 parts.
     Similarly prepared are Ph2CF2, b15 100-1°, n25D 1.5360-1.5368;
     PhCHF2, b15 35-6°; 4-Me2NC6H4CHF2; (FCH2)20; PhCF3 and BzF;
     F3C(CF2)2COF; F3C(CF2)6COF, b. 108-9°; FOC(CF2)3COF, b.
     47-9°; FOC(CF2)2COF, b. 30-5°; 2-F3CC6H4COF and phthaloyl
     fluoride; Me(F2CH)NCOF and Me(HCO)NCOF; Me(MeCF2)NCOF, b. 97-100°
     and MeAcNCOF, b. 136-8°; F2CHNMe2, b. 47-51.5°; PhCF2NMe2,
     b. 63°; N-fluoroformyl-1,1-difluorohexamethyleneimine, b0-5
     50°; and Me2NCF2NMe2, b. 101-3°.
     1963:39841 HCAPLUS <<LOGINID::20071017>>
AN
     58:39841
DN
OREF 58:6752d-f
     Fluorinated organic compounds
TI
     E. I. du Pont de Nemours & Co.
PA
SO
     11 pp.
DТ
     Patent
LA
     Unavailable
FAN.CNT 1
                                DATE
                                          APPLICATION NO.
                                                                  DATE
     PATENT NO.
                        KIND
                                           ______
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                                _____
                                                                  -----
                         ----
                                                                19601109 <--
                                         GB 1960-38526
     GB 909364
                                19621031
PI
                                19651019 US 1959-852939
                                                                 19591116 <--
     US 3213062
PRAI US
                                19591116 <--
     702-99-8P, Benzylamine, \alpha, \alpha-difluoro-N, N-dimethyl-
     RL: PREP (Preparation)
        (preparation of)
     702-99-8 HCAPLUS
RN
CN
     Benzenemethanamine, \alpha, \alpha-difluoro-N,N-dimethyl- (CA INDEX
```

Benzenemethanamine,  $\alpha$ ,  $\alpha$ -difluoro-N, N-dimethyl- (CA INDEX

Ph-CF2-NMe2

NAME)

L10 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN TI The chemistry of sulfur tetrafluoride. II. The fluorin

The chemistry of sulfur tetrafluoride. II. The fluorination of organic carbonyl compounds

GI For diagram(s), see printed CA Issue.

RL: PREP (Preparation) (preparation of) 702-99-8 HCAPLUS

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cf. CA 54, 12862h. In many types of organic compds., the selective AB replacement of O atoms by F can be accomplished with SF4. The replacement reactions are performed by cooling the liquid or solid organic compound O in a Hastelloy-lined vessel under N to -78°, removing the N in vacuo, charging the vessel with the gaseous reactants (HF, BF3, SF4, etc.), heating the sealed vessel for the prescribed period, cooling, venting, and working up by the usual processes of distillation, recrystn., and sublimation (starting material, moles, moles SF4, reaction temperature, reaction time in hrs., product, % yield, and b.p. given): Et-CO2H, 0.60, 1.82, 150°, 8, EtCF3 (scrubbed with 40% aqueous KOH), 89, -; C6H13CO2H, 0.20, 0.65, 130°, 6, C6H13CF3, 80, 101° (n25D 1.3449); C11H23CO2H, 0.33, 2.00, 130°, 6, C11H23CF3, 88, 92°/12 mm. (n25D 1.3896); C17H35CO2H, 0.35, 2.13, 130°, 6, C17H35CF3, 93, 107°/3 mm. (m 28-30°, n25D 1.4148); Me3CCH2CHMeCH2CO2H, 0.19, 0.57, 120°, 6, Me3CCH2CHMeCH2CF3, 64, 121-2° (n25D 1.3657); 4-cyclohexylbutyric acid, 0.20, 0.60, 120°, 10, 1,1,1-trifluoro-4-cyclohexylbutane, 80, 172-3° (n25D 1.3987);  ${\tt CH2\,(CO2H)\,2,\ 030,\ 0.69,\ 40^{\circ},\ 16,\ CH2\,(COF)\,2,\ 70,\ 92-4^{\circ};}$ CH2(CO2H)2, 0.40, 2.40, 150°, 8, CH2(CF3)2 (scrubbed with 40% aqueous KOH), 57, -; (CH2CO2H)2, 0.40, 2.40, 150°, 8, (CH2CF3)2 (scrubbed with 40% aqueous KOH), 41, -; (CH2CH2CO2H)2, 0.67, 2.23, 130°, 7, CF3 (CH2) 4CF3, 19, 99-101° (n25D 1.3519) [and 39% CF3 (CH2) 4CO2H, m. 36-8°]; HO2C(CH2)8CO2H, 0.15, 0.46, 120°, 6, CF3(CH2)8CF3, 27, 90-6°/ 20 (n25D 1.3519) [and CF3(CH2)8COF, 45%, b20 115-18°, and FOC(CH2)8COF, 21%, b20 144-6°]; HO2CCH2CH(CO2H)CH2CO2H, 0.07, 063, 130°, 10, O.CF2.CH2.C-(CF3).CH2.CF2, 20, 104-6°; BrCH2CHBrCH2CO2H, 0.53, 1.85, 140°, 8, BrCH2CHBrCH2CF3, 54, 69-75°/58 mm.; F2CHCF2CO2H, 0.15, 0.48 (and 0.03 mole BF3 as catalyst), 250°, 8, F2CHCF2CF3 (scrubbed with 40% aqueous KOH), 56, - (a run at 180° without catalyst gave only F2CHCF2COF); cyclobutane-1,1-dicarboxylic acid, 0.28, 2.32, 150°, 6, (CF3)2C.CH2.CH2.CH2, 43, 68-9°; CF2.CF2.CF2 CH CH2CO2H, 0.08, 0.30, 160°, 16, CF2.CF2.CF2.CHCH2CF3, 51, 67°; CH2:CHCO2H, 0.75, 2.00, 130°, 8, CH2:CHCF3 (scrubbed with 20 % aqueous KOH), 45, - 26°; CH2: CMeCO2H, 0.75, 2.00, 130°, 8, CH2:C(CF3)Me, 54, 6°; trans-(:CHCO2H)2, 0.55, 2.78, 130°, 9, trans-(:CHCF3)2, 95 (scrubbed with 20% aqueous KOH), 6°; (:CHCH2CO2H)2, 0.10, 0.55, 130°, 10, (:CHCH2CF3)2, 58, 90-1° (n25D 1.3131); CH2:C(CO2H)CH2CO2H, 0.62, 2.80, 160°, 10, CH2:C(CF3)CH2CF3, 26, 47-9° [and 41% CH2:C(COF)CH2CF3, b. 90-5°]; HO2CCH.CH2.CMe:CCO2H, 0.149, 0.89, 120°, 4, CF3CH.-CH2.CMe:CCF3, 31, 95-6° (and 30% CF3CH.CH2.CMe:-CCOF, b. 160-1°); HC.tplbond.CCO2H, 2.00, 2.10, 30-55°, 3, CH.tplbond.CCOF, 28, 22-3°; CH.tplbond.CCO2H, 0.27, 0.78, 120°, 3, CH.tplbond.CCF3 (scrubbed with buffer of pH 8.5 containing 450 g. NaH2PO4.H2O and 220 g. KOH in 4 l. H2O), 60, -; (.tplbond. CCO2H)2 (diluted with 60 g. methylcyclohexane), 0.395, 1.67, 70; 6, (.tplbond.CCOF)2, 51, 40-5°; (.tplbond.CCO2H)2, 0.125, 0.75 (and 0.016 mole TiF4 as catalyst), 170°, 8, (.tplbond.CCF3)2, 80, -; O(CH2CO2H)2, 0.50, 3.00, 130°, 7, O(CH2CF3)2, 35, 58-9° (and O.CH2.CF2.O.CF2.CH2, 14%, b. 91°, n25D 1.3262); EtO2C(CH2)4CO2H, 0.77, 2.00, 130°, 7, EtO2C(CH2)4CF3, 14, 57-9°/11 mm. (n25D 1.3725) [and 13% HO2C(CH2)4CF3, 110-11.5°/17 mm., 37-8.5°]; HOCH2CO2H, 0.75, 3.00,160° 5, FCH2CF3 (scrubbed with 20% aqueous KOH), 48, -26.5° (and 18% FCH2COF, b. 51°); HO2CCH2SO3H, 0.2, 0.69, 180°, 6, CF3CH2SO2F, 41, 105-7°; HO2C(CH2)10SO3H, 0.083, 0.41, 130°, 8, CF3(CH2)10SO2F, 42, 100-10°/0.10 mm.; HO2C(CH2)6CH(CO2H)SO3H, 0.195, 1.61, 150°, 8, CF3(CH2)6CH(CF3)SO2F, 33, 62-4°/0.15; BzOH, 0.25, 0.50, 120°, 6, PhCF3, 22, 100-1° (n25D 1.4133) (and 41% BzF, b. 155-6°); BzCO2H, 0.125, 0.51,100°, 6, PhCF3, 13, 45-55°/ 100 mm. (and 59%

BzF, b100 92-4°); o-C6H4(CO2H)2, 0.10, 0.55, 120°, 6,

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o-C6H4(CF3)2, 43, 140-4° (and o-CF3C6H4COF, 23%, b. 175-8°);
p-C6H4 (CO2H) 2, 0.10, 0.60, 120°, 6, p-C6H4 (CF3) 2, 76,
113-15° (n25D 1.3767) (and 3% p-CF3C6H4COF, b. 156°);
1,2,4,5-C6H2(CO2H)4, 0.07, 0.83, 150°, 6, 1,2,4,5-C6H2(CF3)4, 77, -
(m. 73-4°); p-MeO2CC6H4CO2H, 0.44, 1.33, 130°, 7,
p-MeO2CC6H4COF, 63, 120-1°/ 13 mm. (m. 69-70.5°);
p-O2NC6-H4CO2H, 0.67, 2.12, 130°, 7, p-O2NC6H4CF3, 72, - (m.
41-3°); 4,1,3-ClC6H3(CO2H)2, 0.20, 1.20, 150°, 8,
4,1,3-ClC6H3(CF3)2, 62, 147° (n25D 1.4130); piperazine-2,3,5,6-
tetracarboxylic acid, 0.035, 0.42, 150°, 6, 2,3,5,6-
tetrakis(trifluoromethyl)piperazine, 20, 129°: BzF, 0.145, 0.30
(and 0.05 mole HF as catalyst), 120 °, 6, PhCF3, 41, 100 ^{\circ}
(n24.9D 1.4124); BzCl, 0.20, 0.80, 150 °, 8, BzF, 51, 149°;
BzCl, 0.20, 0.50 (and 0.25 mole HF), 120°, 6, m-ClC6H4CF3, 25,
138-9° (n25D 1.4459); Ac2O, 0.30, 0.20, 300°, 10, MeCF3 (scrubbed with 10% aqueous NaOH), 50, -; maleic anhydride, 0.30, 0.60, 150°, 13, maleic acid difluoride, 71, 100-5°;
dichloromaleic anhydride, 0.20, 0.47, 300°, 10, O.CF2.CC1:CC1.CF2,
46, 73-4°; phthalic anhydride, 0.20, 0.40, 180°, 18,
o-C6H4(COF)2, 93, - (m. 40°); phthatic anhydride, 0.40, 1.60,
350°, 11, o-C6H4(CF3)2, 45, 143°; BzONa (in 100 cc. cyclohexane), 0.25, 0.50, 120°, 6, BzF, 48, 152-5°;
PhC.tplbond.CCO2Na (in 100 cc. cyclohexane), 0.475, 0.52, 45°, 6,
PhC.tplbond.CCOF, 71, 52-3°/2 mm.; BzOMe, 0.30, 0.60, 300°,
6, 55% PhCF3, 98° (and a trace of BzF, b. 151°);
p-C6H4(CO2Me)2, 0.10, 0.60 (and 0.03 mole BF3), 130°, 8,
p-C6H4(CF3)2, 16, 113-16° [and 26% p-CF3C6H4COF, b. 154-8°;
4% p-C6H4(COF)2, m. 122-4°, and a high yield of MeF]; HCO2Me, 0.10,
32 (and 0.05 mole HF), 200°, 6, -, - (high yields of MeF and CHF3
and a low yield of F2CHOMe); MeO2CC:CH.CF2.CF2, 0.20, 0.60 (and 0.03 mole
BF3), 140°, 16, CF3C:CH.CF2.CF2, 10, 42-3°; BzNH2, 0.20,
0.41, 150°, 8, PhCF3, 13, 36-8°/64 mm. (n25D 1.4150);
BzNHMe, 0.25, 0.50 (and 0.05 mole BF3), 60°, 4, BzF, 48,
90-4°/107°; BzNMe2, 0.25, 0.50, 130°, 6, PhCF2NMe2,
17, 70-1°/15 mm. (and 1.3% BzF, b13 50-5°); phthalimide,
0.20, 0.69 (and 0.045 mole BF3), 100°, 10, o-CF3C6H4COF, 58,
176-8°; AcH, 0.60, 0.75, 50°, 14, MeCHF2, 35, above
-34°; C6H13CHO, 0.25, 0.37, 60°, 8, C6H13CHF2,
43,118-19° (n25D 1.3688); \alpha-polyoxymethylene, 2.33, 2.30,
150°, 6, CH2F2, 59, -51-5° [and O(CH2F)2, 21%, b.
32-4°]; H(CF2)4CHO, 0.25, 0.28, 100°, 10, F2CH(CF2)3CHF2,
55, 68-70°; BzH, 0.30, 0.60, 150°, 6, PhCHF2, 81,
130-5° (a similar run but with 0.30 mole SF4 gave no distillable
product); p-C6H4(CHO)2, 0.15, 1.00, 150°, 8, p-C6H4(CHF2)2, 88,
54^{\circ}/20 mm; Me2CO, 0.60, 0.67, 110°, 16, Me2CF2, 60, -10 to
-5°; cyclohexanone, 0.40, 0.41, 39°, 13,
1,1-difluorocyclohexane, 31, 98-9° (n25D 1.3890); BzPh, 0.25, 0.50
(and 0.05 mole HF), 180°, 6, Ph2CF2, 97, 114-15°/7.5 mm.
(n25D 1.5351); BzCF3, 0.075, 0.22, 100°, 8, PhC2F5, 65,
115-16°; Bz2, 0.125, 0.50, 180°, 5, (PhCF2)2, 34, - (m.
122-3°); trioxoindan-H2O, 0.254, 1.55, 120°, 8,
o-C6H4.CF2.CF2.CF2, 25, 34°/4.5 mm. (b70 92-3°);
(EtO2CCH2)2CO, 0.25, 0.50, 80°, 6, (EtO2CCH2)2 CF2, 29,
63-5°/2 mm. (n25D 1.4038); Ac(CH2)2CO2Et, 0.42, 0.48 (and 0.028
mole H2O), 95°, 10, MeCF2(CH2)2CO2Et, 16, 70-2°/27 mm. (n25D
1.3798); BzCH:CHCO2Me, 0.23, 0.48, 160°, 10, PhCF2CH:CHCO2Me, 25,
102-3°/4.5 mm., (n25D 1.4861); p-benzoquinone, 0.20, 0.35 (and 0.35
mole HF), 200°, 4, 1,2,4-C6H3F3, 30, 86.5°; chloranil,
0.14, 0.42 (and 0.15 mole HF), 270°, 2.5, CF2.CC1:CC1.CF2.CC1:CC1,
75, 183-8° (m. 45.5-6.5°) (and 2% CO.CCl:CCl.CF2.CCl:CCl, m.
104-7°); 2,5-dihydroxy-p-benzoquinone, 0.10, 0.55 (and 0.10 mole
HF), 60°, 8, CF2.CF2.CH2.CF2.CF:CH, 40, 88-8.5°;
2-hydroxy-1,4-naphthoquinone, 0.10, 0.50 (and 0.10 mole H2O), 140°,
1.5, 1,1,2,2,4,4-hexafluoro-1,2,3,4-tetrahydronaphthalene, 36,
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91-5°/30 mm.; anthraquinone, 0.059, 0.28, (and 0.05 mole HF),
     225°, 8, 9,9,10,10-tetrafluoroanthracene, 78, - (m.
     122-2.5°); tropolone (I), 0.02 (and 5 cc. C6H6), 0.065, 60°,
     10, 2-fluorotropone, 28, - (m. 74-5°); 3,5,7-tri-Br derivative of I, 0.0033 (and 5 cc. C6H6), 0.02, 60°, 8, 2-fluoro-3,5,7-
     tribromotropone, 57, - (m. 134-42°). CO2 (0.11 mole) and 0.20 mole
     SF4 heated 2 hrs. at 500° yielded 80% CF4 and 10% COF2. COC12 (0.10 mole) and 0.30 mole SF4 in the presence of 0.026 mole TiF4 heated 4
     hrs. at 250° gave 90% CF4 and 9% COF2. CO (0.2 mole), 0.50 mole
     SF4, and 0.5 mole HF heated 7 hrs. at 250° yielded 95% CF4. A
     mixture of 0.75 mole CO and 0.22 mole SOF2 heated 2 hrs. at 500° gave
     70% CO, 13% COS, 6% COF2, and 11% CO2.
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     The chemistry of sulfur tetrafluoride. II. The fluorination of
     organic carbonyl compounds
     Hasek, W. R.; Smith, W. C.; Engelhardt, V. A.
ΑU
     E. I. du Pont de Nemours & Co., Wilmington, DE
CS
     Journal of the American Chemical Society (1960), 82, 543-51
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     CODEN: JACSAT; ISSN: 0002-7863
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